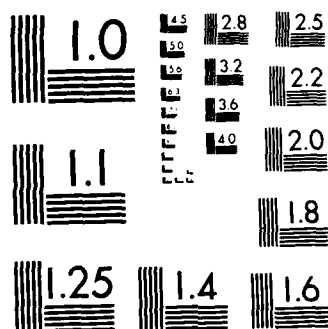


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<p>This research project has investigated topics in unconstrained and constrained optimization, solving systems of nonlinear equations, nonlinear least squares, and parallel optimization. We have continued our development of tensor methods for nonlinear equations and extended these methods to unconstrained optimization and nonlinear least squares. In all cases, the tensor methods appear to provide significant practical improvements over the best currently known methods, on both singular and nonsingular problems. We have developed new trust region methods for equality constrained optimization problems that have strong convergence properties, and have begun to implement these methods. We have also developed new analysis techniques that provide improved local convergence results for constrained optimization problems. We have developed and analyzed an efficient method for "orthogonal distance regression", intended for problems where there are errors in independent as well as dependent variables, and have developed a robust code that implements this method. Finally, we have developed, implemented, and analyzed parallel methods for global optimization and for unconstrained optimization.</p>			
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FINAL REPORT for

ARO Contract DAAG29-84-K-0140
 New Methods for Nonlinear Optimization
 Aug. 1, 1984-Dec. 31, 1987

Principal Investigator: Robert B. Schnabel
 Co-Principal Investigator: Richard H. Byrd

Over the course of this research contract, considerable progress was made in all the areas discussed in the proposal, namely tensor methods for nonlinear equations and unconstrained optimization, local strategies for nonlinearly constrained optimization, globally convergent strategies for nonlinearly constrained optimization, and generalized nonlinear least squares (orthogonal distance regression). We summarize the work in those areas in Sections 1-4. In addition, we have worked on several other topics, namely parallel methods for optimization, and several topics related to unconstrained optimization. This work is summarized in Sections 5 and 6. Section 7 contains a listing of publications and reports supported by this contract, and Section 8 contains a list of research personnel supported by this contract.

1. Tensor Methods for Nonlinear Equations and Unconstrained Optimization.

Under our previous research contract, we had developed a new class of methods, called *tensor methods*, for solving systems of nonlinear equations. This research produced very robust and efficient general purpose methods that are especially effective for solving singular problems. Tensor methods were first developed for solving nonlinear equations problems where the Jacobian is available at each iteration, as in Newton's method. This method augments the standard linear model, the first two terms of the Taylor series, by a low rank, second order tensor term which is chosen to allow the model to interpolate some function values at previous iterates. This is done in such a way that the cost of forming, storing, and solving the model is not significantly higher than for Newton's method. In extensive computational tests, this tensor method was considerably more efficient than a standard algorithm based on Newton's method, with average gains of about 40% on the harder test problems where $F'(x^*)$ is nonsingular, and gains of around 60% and 50% on the harder problems where $\text{rank } F'(x^*) = n-1$ or $n-2$ respectively. This work is described in a paper by Schnabel and Frank published in the *SIAM Journal on Numerical Analysis*, and forms a portion of Frank's Ph.D thesis.

We also developed a tensor method for nonlinear equations for situations where, as in Broyden's method, Jacobians are unavailable and the algorithm is based solely on function values at the iterates. It is more difficult to make effective use of a second order term in this case, but this tensor method still produced average gains of about 10% on nonsingular problems, and about 25% and 33% when $\text{rank } F'(x^*) = n-1$ or $n-2$, respectively. The secant tensor method is described in Frank's Ph.D thesis, and in a paper by Schnabel and Frank in *The State of the Art in Numerical Analysis*, M.J.D. Powell and A. Iserles, eds.

Our main accomplishment in tensor method research under this contract has been to successfully extend tensor methods to unconstrained optimization problems. This research has been conducted with a Ph.D student, Ta-Tung Chow, who has been supported by this contract. The extension of tensor methods to unconstrained optimization is not straightforward. We have first considered the case when the Hessian matrix is available, and have used a fourth order tensor model, rather than a third order model which

would be the analog of the nonlinear equations case. The reasons for using a fourth order model are that a third order model will be unbounded below, and that fourth order information is needed to accelerate convergence on singular problems. We form this model by interpolating the function and gradient values at previous iterates; in practice it seems that it is only effective to interpolate the information from the most recent past iterate. The additional cost of forming, storing, and solving this model is not significant in comparison to the standard cost of Newton's method. In our experiments, the tensor method is considerably more efficient than a comparable method based on quadratic models, with average savings of at least 30% on both non-singular and singular problems. This research has been presented at several conferences, and in Chow's M.S. thesis, and is currently being prepared for publication.

Recently we have begun work on applying tensor methods for unconstrained optimization to secant methods, where the Hessian matrix is approximated from gradient (and function) values. This will be one of our main projects under our new ARO contract. Both tensor method projects will be included in Chow's Ph.D thesis.

We have also continued to develop tensor methods for nonlinear equations along with another graduate student, Ali Bouaricha. We have extended the method to nonlinear least squares problems, and developed a high quality piece of software that solves both nonlinear equations and nonlinear least squares problems by tensor methods. This code also uses a trust region method where earlier research used a line search. This research is described in Bouaricha's M.S. thesis, and is being prepared for publication.

2. Local strategies for nonlinearly constrained optimization.

Most of our research on local strategies has involved reduced Hessian methods for constrained optimization. By this, we refer to successive quadratic programming methods where only the Hessian of the Lagrangian with respect to the null space of the constraints is approximated. We have made a serious study of the use of a second order correction step of the type proposed by Roger Fletcher in conjunction with reduced Hessian methods. A paper by Richard Byrd showing that such a correction results in a better asymptotic convergence rate has appeared in *SIAM Journal on Numerical Analysis*. This paper also shows that a similar improvement can occur with standard SQP methods. We have also done computational testing on the effect of a second order correction step with several constrained strategies.

A problematic issue in using the reduced Hessian is the choice of basis for the null space. We have mathematically investigated the issue of continuity of the null space basis and shown that such continuity is impossible to attain globally in most cases. We have also devised an algorithm that avoids the discontinuity difficulties by making the reduced Hessian method independent of basis choice. A paper describing this work, by Richard Byrd and Robert Schnabel, has appeared in *Mathematical Programming*.

Although we and others have made progress on secant methods for nonlinearly constrained optimization, there is a lack of understanding of the behavior of these methods except very close to the solution. Therefore we have decided to try to extend the somewhat global results of Powell on convergence of the BFGS method with arbitrary starting Hessian in the convex case to some constrained methods. Our first achievement along these lines is to extend Powell's result for the BFGS method to the restricted Broyden class except for the DFP. This work has been described in a paper by Richard Byrd, Jorge Nocedal and Ya-Xiang Yuan published in *SIAM Journal on Numerical Analysis*.



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3. Globally convergent strategies for nonlinearly constrained optimization.

Work in this area has concentrated on trust region methods for nonlinearly equality constrained problems. In unconstrained optimization trust regions have proven to be effective devices for guaranteeing convergence to the solution of optimization problems from poor starting points. We have devised an algorithm which uses trust regions in conjunction with successive quadratic programming for which we can prove the standard global convergence results without any assumption of positive definiteness of the Hessian approximations. In addition, we can guarantee that the limit point satisfies second order optimality conditions (the first time this has been shown for a nonlinearly constrained optimization algorithm), and that no Maratos type effect can cause the trust region to interfere with rapid local convergence. Unfortunately the method is still sensitive to near linear dependence of the constraint gradients. This is a serious defect, which is shared by almost all methods for nonlinearly constrained optimization. These theoretical results have been presented in a paper by Richard Byrd, Robert Schnabel, and Gerald Shultz of Metropolitan State College in Denver in *SIAM Journal on Numerical Analysis*. The method has been implemented with the aid of Emmanuel Omojokun, a Ph.D. student in this department. We have made several improvements to the algorithm and the initial experimental results are encouraging.

4. Generalized nonlinear least squares.

By generalized nonlinear least squares we mean a generalization of standard least squares in which random errors are assumed to occur in all model variables. We also refer to this approach as orthogonal distance regression (ODR). We have first considered the case of this problem where the model is given by an explicit formula. Although the number of variables in the problem is proportional to the number of data points, we have devised a Levenberg-Marquardt type algorithm in which the work per step is only linear in the number of data points. A program implementing this algorithm has been used on several fitting problems arising from engineering applications, and an analysis has been done of its convergence. A paper by Paul Boggs of NBS, Richard Byrd, and Robert Schnabel describing and analyzing our algorithm and giving test results has appeared in *SIAM Journal on Scientific and Statistical Computing*. In addition a paper on the algorithm has appeared in the proceedings of the Eighteenth Symposium on the Interface of Computer Science and Statistics. With the help of Janet Donaldson of NBS the algorithm has been implemented in a good quality software package, ODRPACK, and a paper by Paul Boggs, Richard Byrd, Janet Donaldson and Robert Schnabel has been submitted to *ACM Transactions on Mathematical Software*. This package has already attracted over 20 users around the country and the world.

As a byproduct of analyzing this algorithm we have been able to derive some new results on local behavior of trust region algorithms. Specifically we have been able to show that a standard trust region strategy using a bounded Hessian approximation converges linearly if it converges. This implies linear convergence of the More implementation of the Levenberg-Marquardt algorithm, for example. We are currently writing up this research.

We have also completed a statistical comparison of our ODR method to standard nonlinear least squares on a number of models, in cases when there is experimental error in all model variables. The study indicated that the estimates produced by ODR were as good or better than those produced by standard nonlinear least squares in all the cases we tested. A paper on this research by Paul Boggs, Janet Donaldson, Robert Schnabel, and Clifford Spiegelman of NBS has appeared in the *Journal of Econometrics*.

5. Parallel Methods for Optimization.

During this research period, we have become strongly interested in parallel computation, especially parallel methods for optimization. A general discussion of this subject is given in a paper by Schnabel in *Computational Mathematical Programming*, K. Schittkowski, ed. One contribution to parallel optimization during this period has been the construction of a parallel stochastic global optimization method and the implementation and testing of this method on a network of Sun workstations. This work was conducted jointly with A. Rinnooy Kan of Erasmus University and his student C. Dert, who spent nine months at the University of Colorado. It is described in a paper by Byrd, Dert, Rinnooy Kan, and Schnabel that will appear in the proceedings of the ARO Workshop on Parallel Processing and Medium-Scale Multiprocessing, and in a paper that has just been accepted for publication in *Mathematical Programming*.

We have also developed parallel methods for unconstrained optimization during this period. A paper by Schnabel in *Computer Methods in Applied Mechanics and Engineering* proposes several parallel methods for problems with expensive function evaluations and discusses their performance. A paper by Byrd, Schnabel, and Shultz in *Annals of Operations Research* motivates cases where one might evaluate part, but not all, of the Hessian matrix at each iteration in parallel optimization, and proposed, analyzes, and tests several ways to do this. Another paper by Byrd, Schnabel, and Shultz that has been tentatively accepted for publication in *Mathematical Programming* continues the development of these methods, and also discusses the efficient parallel implementation of the linear algebraic operations in secant methods for unconstrained optimization.

We also developed some software tools to facilitate the use of a network of workstations as a distributed memory multiprocessor. This system, called DPUP, is described in a paper by Gardner, Gerard, Mowers, Nemeth, and Schnabel in *SIGNUM Newsletter*, and has been distributed to a number of other sites.

6. Other Research Topics in Unconstrained Optimization.

A project begun under the previous research contract on computational experiments with trust region methods for unconstrained minimization was completed. This involved computation of trust region steps by minimizing the quadratic model on a two dimensional subspace within the trust region. A paper on this work by Byrd, Schnabel and Gerald Shultz has appeared in *Mathematical Programming*.

The techniques used by Byrd and Nocedal in analyzing the convergence of constrained optimization methods are of substantial interest in unconstrained optimization as well. A paper by Byrd and Nocedal discussing some of these issues has recently been submitted to *SIAM Journal on Numerical Analysis*.

A crucial part of most line search codes for unconstrained and constrained optimization is the modified Cholesky decomposition of Gill and Murray. We have developed a new modified Cholesky decomposition that has superior theoretical properties to existing methods, and appears to perform better in practice as well. This research has been presented at a conference and is being readied for publication.

Finally, John Dennis of Rice University and Robert Schnabel completed an extensive survey of methods for unconstrained optimization, which will appear in *Handbooks in Operations Research and Management Science, Vol. 1, Optimization*.

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Students Supported by Contract DAAG29-84-K-0140

(P.D. Frank, supported under previous contract, Ph.D awarded, August 1984)

T. Gardner, research assistant, Aug 1984 - May 1985

T. Chow, research assistant, June 1985 - Dec 1987
M.S. awarded, May 1986 (now working for Ph.D)

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